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1. Introduction

Since our laboratory was set up in the Institute, the fundamental and theoretical researches have been performed in the field of physics, associated with chemistry, but our interest is being directed to fundamental problems of biology besides the above-mentioned subjects. The principal methods of our investigations are quantum mechanics and group algebra in generalized meaning, and especially the latter is not only very advantageous in the treatment of the so-called many-body problem in quantum mechanics, but also it is expected to obtain some foundations and further extensions of quantum mechanics from the modern algebraic point of view; while recent experimental researches with remarkable accuracy of microwave and radiowave spectra have called our attention to the subject of nuclear electromagnetic interactions with an outer charged system. These problems must give us some phenomenological knowledge of nuclear structures with high accuracy by means of hyperfine structures of atoms and molecules. Recent researches attained with the above object in view in our laboratory will be generally reviewed in the following.

2. The Foundation of Classical Electrodynamics

Maxwell's phenomenological theory and Lorentz's electron theory of classical electrodynamics have to be corrected in regard to the following essential incompleteness from the view-point of the primary quantum electrodynamics:

1. The microscopic electromagnetic field quantity itself cannot be expressed by a point function in terms of the classical theory of the electron, but it must be represented by an incommutable operator in general.

2. The microscopic electric charge density as well as current density must be expressed by a formula derived from quantized wave functions.

Due to the above consideration Dr. Yukawa has given the quantum-mechanical foundation of classical electrodynamics—the foundation of *observability* of the macroscopic electromagnetic field in terms of Heisenberg-Pauli's theory, and that of *macroscopic average* of electric charge or current density by non-relativistic quantum theory of the electron system, and he has shown what approximation of the quantum-mechanical treatment the classical theory can be justified for¹⁾.

We can find in his paper that as to the first problem the macroscopic electromagnetic field \mathbf{E}, \mathbf{B} has enough to be considered as an ordinary vector function, so far as the field strength is large enough to be measured in the macroscopic sense.

With regard to the second problem we know the fact that the Lorentz formula can be obtained enough for the approximation of setting aside the spin of the electron and the interaction of the electron with the electromagnetic field. But it is noted that these considerations are of importance in the correspondence-theore-

tical meaning, indifferent to the modern quantum electrodynamics or the non-local field theory for himself.

3. Transformation Properties of the General Spin-Wave System

When we want to treat a complex physical system by quantum mechanics, we cannot but meet frequently with the so-called many-body problem. Above all, in the eigenvalue problem of a system including several identical particles, e. g. nuclear, atomic, or molecular system, the approximation of dealing with every system as an ensemble of several similar sub-systems, each containing one or several nucleons or electrons—the so-called one-body approximation—can be sometimes effective, in order to determine the states of any total system. In particular there are some methods for the many-electron system, each elementary particle having the spin value of $\frac{1}{2}\hbar$. One of these methods has been developed by Racah²⁾ during the war-time, while recently Dirac's character operators have been evaluated for higher permutations on the line of his original program³⁾.

Such being the case we have attempted to find the transformation of spin functions of a system composed of several identical sub-systems, each having a higher spin value. In order to generalize and simplify our problem, we have treated them by the method of the group representation⁴⁾. According to the method, the results in view have been obtained by performing the simultaneous reduction of both the representations of the rotation and symmetric groups regarding the spin functions as the bases^{5) 6)}. The general construction of the spin functions has also been given for appropriate linear combinations of the unitary basic vectors of each spin space⁷⁾.

This method with the results has been applied to the nuclear resonance phenomena in the molecular system^{8) 9)}, whose extensions lead to the quantum-statistical foundation of the classical symmetry number of the molecule¹⁰⁾, and to the general determination of the quantum weights of the allowed energy levels, defining the *nuclear spin isomerism*¹¹⁾. At the same time the molecular partition function is generally constructed from the standpoint of quantum statistics¹²⁾.

Further applications have become possible to the problem not only of the nuclear spin degeneracy (without resolving the nuclear spin multiplicity), but also to that of the nuclear quadrupole coupling, the nuclear magnetic interaction in the molecular or crystalline system, or of the nuclear shell structure composed of the nucleon system¹³⁾.

4. The Problem of Degeneracy in Quantum Mechanics

In general quantum-mechanical investigations, as well-known, the problem of degeneracy of energy spectra plays an important role. This degeneracy is associated with the symmetry condition under which the Hamiltonian is invariant, and is related not only to the three-dimensional rotation group and the symmetric permutation group which produces the so-called *permutation degeneracy*, but also to the symmetry group in a broad sense. The problem stated in the previous section belongs to the former type of degeneracy. The latter is, for example, based upon the fact that even the Schrodinger equation for the hydrogen atom

actually has the symmetry of the four-dimensional rotation group for the negative energy (bound) states, and the symmetry of the Lorentz group for the positive energy (continuous) states. In this case there is an attempt of generalizing the degeneracy problem, which is related to the existence of groups of contact transformations, and of developing the correspondence between the transformations in classical and quantum mechanics¹⁴⁾.

We have attempted to find more fundamental foundation and some possible extensions of this problem. As a preliminary survey the representation of the infinitesimal rotation in the multi-dimensional space has been obtained¹⁵⁾, and at the same time by extension to the system of an isotropic oscillator, we have been able to determine the energy levels from the general point of view concerning the present problem.¹⁶⁾ The essential part of this subject keeps going to be investigated.

Now let us consider a fundamental example of the n -dimensional harmonic oscillator:

$$H = \sum_{\lambda=1}^n \frac{1}{2} (p_{\lambda}^2/m + kq_{\lambda}^2),$$

then the integrals commutable with H are as follows:

$$\begin{aligned} F_{(\lambda)}^{\lambda'} &= (i\hbar)^{-1} (q_{\lambda'} p_{\lambda} - q_{\lambda} p_{\lambda'}), \\ \tilde{F}_{(\lambda)}^{\lambda'} &= (i\hbar\sqrt{mk})^{-1} (p_{\lambda'} p_{\lambda} + mkq_{\lambda'} q_{\lambda}), \\ G_{(\lambda)} &= (2i\hbar\sqrt{mk})^{-1} [(p_{\lambda'}^2 - p_{\lambda}^2) + mk(q_{\lambda'}^2 - q_{\lambda}^2)], \end{aligned}$$

where $1 \leq \lambda' \leq \lambda - 1$. If we denote by $\mathfrak{N}_{(\lambda)}$ the whole integrals of the sub-indices $\leq \lambda$ in F , \tilde{F} , and G , it is shown that $\mathfrak{N}_{(\lambda)}$ is a set of the operators of infinitesimal transformations belonging to the λ -dimensional unimodular unitary group, to wit, it makes a base of the Lie ring, and further it is isomorphic with the Lie ring made from the characteristic matrices of the group mentioned above. From these results we can immediately understand that the group generated by $\mathfrak{N}_{(\lambda)}$ is isomorphic with the λ -dimensional unimodular unitary group with (λ^2-1) -parameters, and so the Schroedinger group of the n -dimensional harmonic oscillator is isomorphic with the above group in case of $\lambda=n$.

5. Interaction between Nuclear-Vibrational and Electronic States

In the preceding sections we treated of quantum-algebraic problems, which have an important signification in the general foundation of quantum mechanics. In the present and the following sections we shall treat some special subjects. At first the spectroscopy of short wave length region, associated with electronic transitions in general, have given us the question of the incomplete separation of electronic and vibrational states in terms of Born-Oppenheimer's theory¹⁷⁾.

Jahn and Teller gave the proof of the general theorem: all degenerate electronic states, without special two-fold one, of non-linear nuclear configurations in the polyatomic molecules are unstable whether the degeneracy is due to electronic orbitals or to spin. Only the linear configurations in degenerate electronic states can be, however, stable with respect to all displacements of the nuclei. Since

orbital two-fold degeneracy is essentially due to the axial symmetry of the nuclear configuration, they may split by breaking their linearity, e. g. the nuclear displacements of the normal mode of a deformation vibration, and it is expected that the magnitude of the splitting of their levels becomes the same order of magnitude as the potential energy of the nuclear vibration. Under these conditions, therefore, we have had to reconsider the ordinary separation into the electronic and nuclear motions¹⁸⁾.

The wave function of a linear nuclear configuration can be given by

$$\Psi(\mathbf{q}_n, \mathbf{q}_e) = \chi^+(\mathbf{q}_n) \psi_n^+(\mathbf{q}_e) + \chi^-(\mathbf{q}_n) \psi_n^-(\mathbf{q}_e),$$

where $\psi_n^+(\mathbf{q}_e)$ and $\psi_n^-(\mathbf{q}_e)$, belonging to the eigenvalues $E_n^e \pm \sigma(r)$, are respectively symmetric and antisymmetric electronic functions for the reflection by the plane containing the principal axis, and $\sigma(r)$ principally determined by perturbation calculation is the half value of the electronic separation which gives the magnitude of the interaction between the electronic and nuclear motions. So we can obtain the following Schrodinger equation for the two-dimensional vector \mathbf{X} , whose components are the nuclear functions $\chi^+(r, \phi)$ and $\chi^-(r, \phi)$ mentioned above:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{\partial}{\partial \phi} - \Lambda \mathbf{P} \right)^2 \right] \mathbf{X}(r, \phi) + \frac{2\mu}{\hbar^2} [E - E_n^e + \mathbf{Q} \cdot \boldsymbol{\sigma}(r)] \mathbf{X}(r, \phi) = 0$$

with

$$\mathbf{P} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \mathbf{Q} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

where Λ (unit by \hbar) is the electronic angular momentum about the principal axis, μ being the reduced mass of this vibration. From the fundamental equation and the perturbation calculation it has been shown that the vibrational structure can be determined in relation to the electronic Π - Λ transition.

6. The Theory of Hyperfine Structures

Experimental researches with remarkable accuracy have recently progressed in long wave length—microwave and radiowave—region. Due to these accurate results we have become possible to formulate critically the nuclear electromagnetic interactions with an outer charged system¹⁹⁾. These problems have given us some phenomenological knowledge of nuclear structures through the theory of hyperfine structures of atoms and molecules.

In the first place let us pay attention to the most fundamental system containing the deuteron, which has a nuclear structure with the magnetic dipole and electric quadrupole moments. How does this nuclear structure affect the hyperfine structure of the deuterium atom or molecule? Now we consider the system composed of two nucleons—a proton and a neutron—and an outer electron (the deuterium system), then our fundamental wave equation, including the effect of exchange forces between the two nucleonic states, is as follows²⁰⁾:

$$\begin{aligned}
& [(E - c\boldsymbol{\alpha} \cdot \mathbf{p}_e - \beta mc^2) + \frac{\mathbf{p}_1^2}{2M_1} + \frac{\mathbf{p}_2^2}{2M_2} + W] \psi(\mathbf{r}_1 \mathbf{s}_1; \mathbf{r}_2 \mathbf{s}_2) \rho - \phi(\mathbf{r}_e) \\
& = [J_W(\mathbf{r}) \psi(\mathbf{r}_1 \mathbf{s}_1; \mathbf{r}_2 \mathbf{s}_2) + J_H(\mathbf{r}) \psi(\mathbf{r}_2 \mathbf{s}_2; \mathbf{r}_1 \mathbf{s}_1) J_M(\mathbf{r}) \psi(\mathbf{r}_2 \mathbf{s}_1; \mathbf{r}_1 \mathbf{s}_2) \\
& \quad + J_B(\mathbf{r}) \psi(\mathbf{r}_1 \mathbf{s}_2; \mathbf{r}_2 \mathbf{s}_1) + T(\mathbf{r}, \sigma_1 \tau_2) J_T(\mathbf{r}) \psi(\mathbf{r}_1 \mathbf{s}_1; \mathbf{r}_2 \mathbf{s}_2) \\
& \quad + V(\mathbf{r}_1 \tau_1; \mathbf{r}_2 \tau_2) \psi(\mathbf{r}_1 \mathbf{s}_1; \mathbf{r}_2 \mathbf{s}_2)] \rho - \phi(\mathbf{r}_e),
\end{aligned}$$

where \mathbf{r}_e is the coordinates of the electron from the origin (the center of gravity of the two nucleons); \mathbf{r}_i and $\sigma_i = 2\mathbf{s}_i$ ($i=1,2$) are respectively the orbital and spin coordinates of the nucleons, especially \mathbf{r} being the relative coordinates of them. $J(\mathbf{r})$ is the short range interaction potentials, and interaction operator:

$$T(\mathbf{r}; \sigma_1 \sigma_2) = -3 \frac{(\mathbf{r} \sigma_1)(\mathbf{r} \sigma_2)}{r^2} + (\sigma_1 \sigma_2)$$

is based upon the tensor force. The electrostatic interaction between the nucleons and the electron:

$$V(\mathbf{r}, \mathbf{r}_e, \tau_1 \tau_2) = -\frac{e^2(1 - \tau_z^{(1)})}{2|\mathbf{r}_e - \mathbf{r}/2|} - \frac{e^2(1 - \tau_z^{(2)})}{2|\mathbf{r}_e + \mathbf{r}/2|}$$

produces the following equation, excluding the only part of the nuclear motion:

$$(E - c\boldsymbol{\alpha} \cdot \mathbf{p}_e - \beta mc^2) \psi(\mathbf{r}, \mathbf{s}) \rho - \phi(\mathbf{r}_e) = V(\mathbf{r}, \mathbf{r}_e, \tau_1 \tau_2) \psi(\mathbf{r}, \mathbf{s}) \rho - \phi(\mathbf{r}_e),$$

where ρ is the antisymmetric change function, τ the isotopic spin operator. Now integrate about \mathbf{r} , \mathbf{s} , and τ , then we get

$$\begin{aligned}
(E - c\boldsymbol{\alpha} \cdot \mathbf{p}_e - \beta mc^2) \cdot \phi(\mathbf{r}_e) &= -\frac{1}{2} e^2 \left[\int d\mathbf{r} \psi^*(\mathbf{r}) \psi(\mathbf{r}) / |\mathbf{r}_e - \mathbf{r}/2| \right. \\
&\quad \left. + \int d\mathbf{r} \psi^*(\mathbf{r}) \psi(\mathbf{r}) / |\mathbf{r}_e + \mathbf{r}/2| \right] \phi(\mathbf{r}_e),
\end{aligned}$$

where $\phi_0(\mathbf{r}_e)$, the zero-th order solution in regard to the *point-model* nucleus, is nothing but the Dirac function for the ground state of the hydrogen atom. By solving the above equation for an appropriate approximation of the nuclear force, we can obtain the electronic function, which makes us possible to calculate the magnetic field \mathbf{H}_0 generated at the origin by the outer electron. The magnetic interaction energy in question is given by the product of \mathbf{H}_0 and the magnetic moment of the deuteron itself.

The present theory is expected to refine not only, to be sure, Fermi's theory²¹⁾, but also, in principal, Bohr-Low's theory^{22), 23)} based upon the model of the neutron rotating with the proper magnetic moment about the proton at the origin. And from our theoretical point of view, the nuclear quadrupole interaction, where the tensor force plays an important role, has also been given a reasonable foundation, but their numerical criticism will be discussed later.

As the next step of this problem we want to evaluate the electric quadrupole moment of the nucleus Li^7 by the theory of the nuclear shell structure as well as the hyperfine structure of the LiH molecule. So it is expected that the quadrupole coupling constant of the molecule will be determined experimentally in the near future.

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